LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

LLNL-TR-525083

Level-2 Milestone 4468: *Lorenz Simulation Interface Beta Release*

Milestone Report for NNSA HQ

Prepared by Jeffery Long and Joel Martinez
December 21, 2011

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Contents

Introduction

This report documents LLNL Lorenz project activities related to simulation web interfaces, ASC L2 milestone NNN: Lorenz Simulation Interface Beta Release, due December 31, 2011. The full text of the milestone is included in Attachment 1. The description of milestone is:

> *This milestone builds upon the Lorenz HPC job management application, a web-based tool for submitting and managing batch jobs. FY12 work will encompass the following new Lorenz deliverables: 1) a web-based interface for specifying and launching a vertical application of interest to ASC, and 2) the associated web service infrastructure for supporting these operations. The Lorenz project is focused on making HPC easier and more efficient through the use of state-of-the-art web technologies..*

The milestone was completed on December 21, 2011 when a fully functional web interface to pre-defined ParaDiS simulations was made available to beta users. Gregg Hommes from the ParaDiS team successfully specified, customized, and submitted a ParaDiS simulation on an LC system through the Lorenz web interface.

A letter certifying that the ParaDiS code team verified correct and complete operation of the Lorenz simulation interface is included as Attachment 2. An overview of the Lorenz system architecture is included as Attachment 3. Screen captures of the Lorenz simulation interface are provided in Attachment 4.

Lorenz Project Overview

The goal of Lorenz is to develop a sophisticated web-based framework as a front end to Livermore Computing Center resources. The primary features include: a personalized dashboard for each user, giving an at-a-glace overview of all computing center resources; a front-end to job submission and management; and a software framework to extend the convenience of web interfaces into simulation codes, including support for setting up, launching, steering, and monitoring simulations.

Because the breadth of desktop operating systems in use both inside and outside LLNL spans all flavors of Linux, Mac, and Windows, the decision was made to use exclusively web-based technologies in Lorenz. Recent advancements in AJAX and Javascript programming, along with coming advances in the form of HTML5 and CSS3, made the browser the preferred development platform. The goal is to provide the user with a robust application interface that requires nothing more than a modern, standards-based web browser. This approach not only provides convenient access to Lorenz for internal and external users, but also has significant advantages over conventional applications in terms of rapid deployment and updates.

The first phase of the Lorenz project is a system “dashboard”, known as MyLC, that gives LC users a rich set of portal applications, or “portlets”, from which to choose. Information that previously required knowledge of dozens of different commands, files, and web pages is now available in one convenient location. This includes account information, bank and disk usage, quotas, cluster utilization, news items, active jobs on LC systems, and more. The extensible software design of the dashboard allows users and staff members to develop their own portlets, and for them to be shared with all users or just within work groups.

The second major phase of Lorenz was built on the idea that HPC centers are managed around batch processing, and “jobs” (or “runs”) progress through several discrete stages: setup, submission, queuing/waiting, running, completion, analysis, and archiving. Lorenz aims to ultimately tie all of these pieces together, including integration with the dashboard and application portals. In addition to helping guide users through the process of defining batch parameters, monitoring job progress, and interacting with jobs and job output, Lorenz also aims to promote access to additional tools and capabilities which to this point have been limited to use by power users. Ultimately Lorenz will assist users in choosing the appropriate resources, such as cluster and file system, given the requirements of a job.

The third major phase of Lorenz, the subject of this milestone, is the development of an application portal. This involves teaming with application codes to provide a simple graphical interface to the simulations, which in turn seamlessly ties into job submission and monitoring. This will allow users to directly define simulation parameters and launch applications using a simple but powerful web front-end.

Because many complex multi-physics codes can have thousands of inputs, providing a general GUI for building an input deck from scratch is impractical. However, most users of large applications start with an existing input file, and make some number of small changes to it. The application portal will feature a process that combines trusted and

validated input files with a GUI that guides the user toward making the relatively minor changes needed for their particular problem. The input files will be in the form of templates, containing most of the data needed for a particular problem along with parameterization of changeable inputs. For expert users, there ultimately will be a way to edit the final input file directly - in the event that there are input changes needed that were not captured in the GUI.

Attachment 1: Milestone Definition Text

<table>
<tr><th colspan="4">Milestone (4468): Lorenz Simulation Interface Beta Release</th></tr>
<tr><td>Level: 2</td><td colspan="2">Fiscal Year: FY12</td><td>DOE Area/Campaign: ASC</td></tr>
<tr><td colspan="4">Completion Date: 12/31/11</td></tr>
<tr><td colspan="4">ASC nWBS Subprogram: CSSE</td></tr>
<tr><td colspan="4">Participating Sites: LLNL</td></tr>
<tr><td colspan="4">Participating Programs/Campaigns: ASC</td></tr>
<tr><td colspan="4">Description: This milestone builds upon the Lorenz job management application, a Web-based tool for submitting and managing batch jobs. FY12 work will encompass the following new Lorenz deliverables: 1) a Web-based interface for specifying and launching a vertical application of interest to ASC, and 2) the associated Web service infrastructure for supporting these operations. The Lorenz project is focused on making HPC easier and more efficient through the use of state-of-the-art Web technologies.</td></tr>
<tr><td colspan="4">Completion Criteria: This milestone is complete when users are able to use the Lorenz Web application to populate a simulation input deck, as well as launch and monitor jobs on both the classified and unclassified networks at LLNL.</td></tr>
<tr><td colspan="4">Customer: SSP and weapons science customers.</td></tr>
<tr><td colspan="4">Milestone Certification Method:
Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion.
The “handoff” of the developed capability (product) to a nuclear weapons stockpile customer is documented.</td></tr>
<tr><td colspan="4">Supporting Resources: LC Division personnel and ASC customers.</td></tr>
<tr><td colspan="4">Supporting Milestones:</td></tr>
<tr><td>Program</td><td colspan="2">Title</td><td>Due Date</td></tr>
<tr><td>N/A</td><td colspan="2"></td><td></td></tr>
<tr><td colspan="4">Codes/Simulation Tools Employed: None</td></tr>
<tr><td colspan="4">Contribution to the ASC Program: Improved ability to manage, monitor, and launch simulation jobs running on ASC supercomputers.</td></tr>
<tr><td colspan="4">Contribution to Stockpile Stewardship: Improved ability to manage, monitor, and launch simulation jobs running on ASC supercomputers.</td></tr>
</table>

Milestone (4468): Lorenz Simulation Interface Beta Release				
No.	**Risk Description**	**Risk Assessment (low, medium, high)**		
		Consequence	**Likelihood**	**Exposure**
1.	Schedule slips	Low	Low	Low

Attachment 2: Handoff Letter

December 22, 2011

To: Michel McCoy, LLNL ASC Program Leader
From: Gregg Hommes
Subject: Completion of ASC Level 2 Milestone 4468

I certify that the Lorenz simulation interface for the ParaDiS application has been made available as a beta release. Multiple pre-defined simulation options are available to users, including copper and tantalum. Using the Lorenz web interface, simulation input parameters of interest to users can be modified, and jobs can easily be submitted to LC HPC resources.

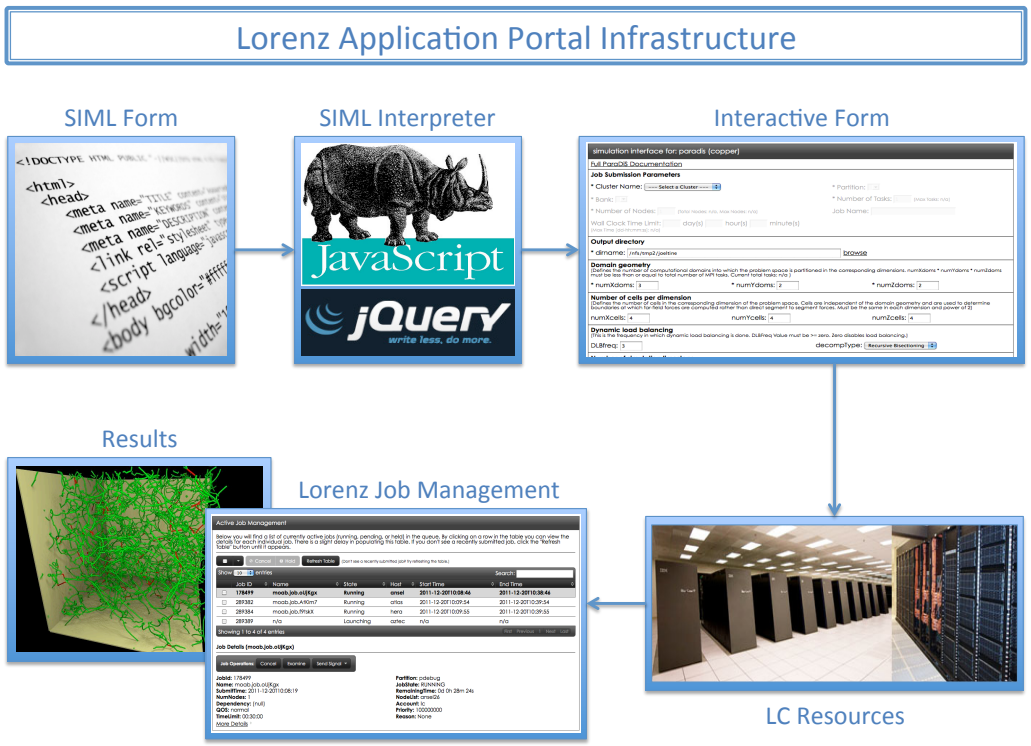
The beta release of the Lorenz simulation interface capability meets the milestone completion criteria for L2 Milestone 4468, Lorenz Simulation Interface Beta Release.

Gregg Hommes

Gregg Hommes
ParaDiS Code Developer

Lawrence Livermore National Laboratory

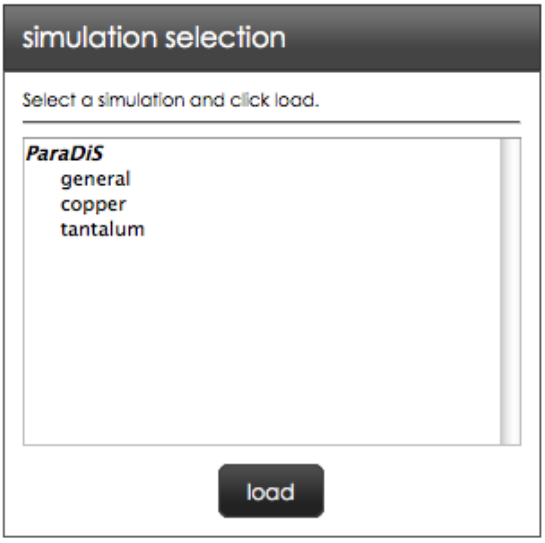
Attachment 3: The Lorenz Application Portal Architecture



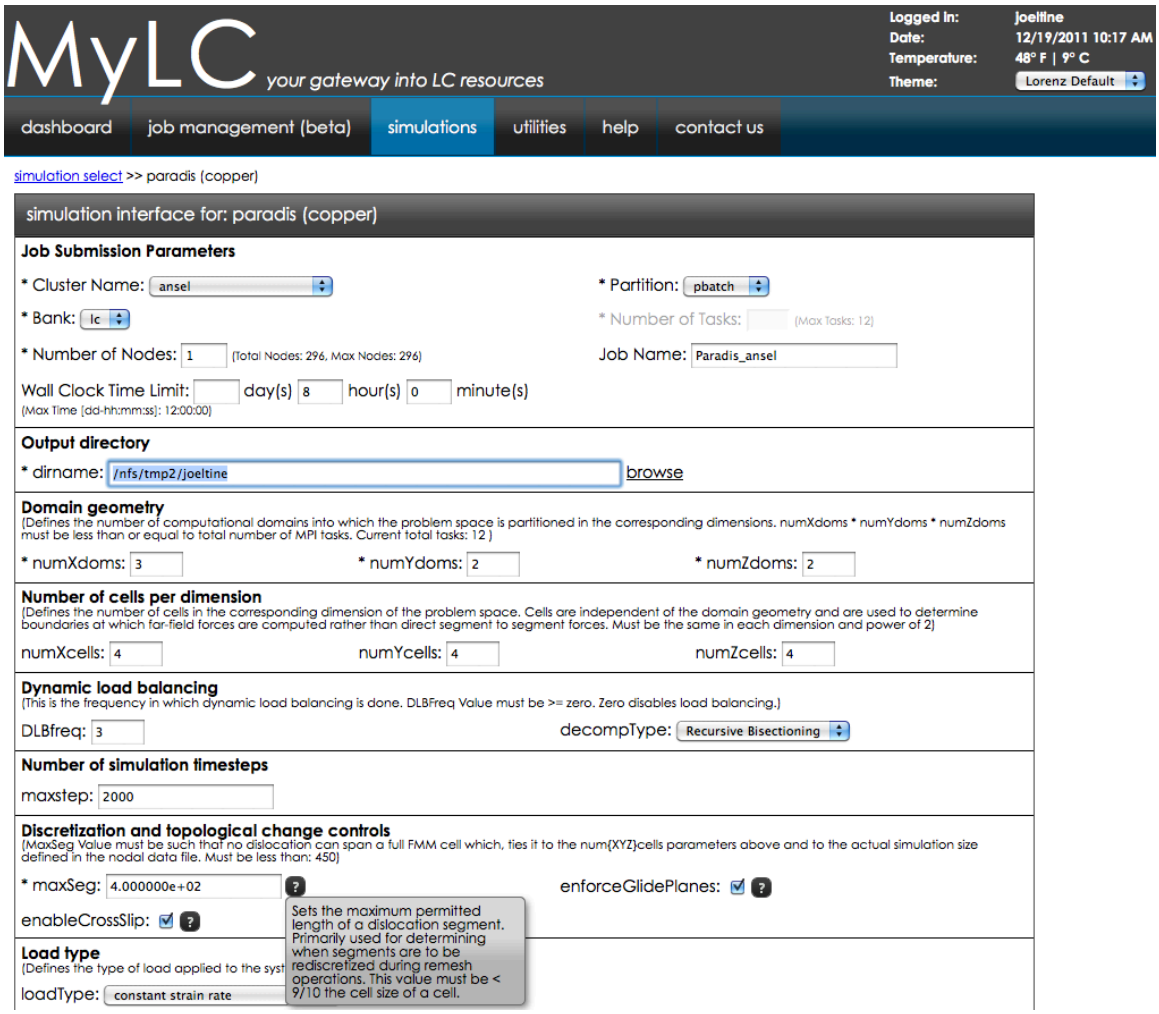
Lorenz System Architecture for the Application Portal

The Lorenz application portal makes use of forms written in the Simulation Input Markup Language (SIML). These forms are interpreted into HTML format and presented in the user's web browser. After completing and submitting the form, simulation input files are created on an LC resource, and a batch job is submitted. The user is directed to the Lorenz job management element to monitor progress, as well as to examine the results of the completed simulation.

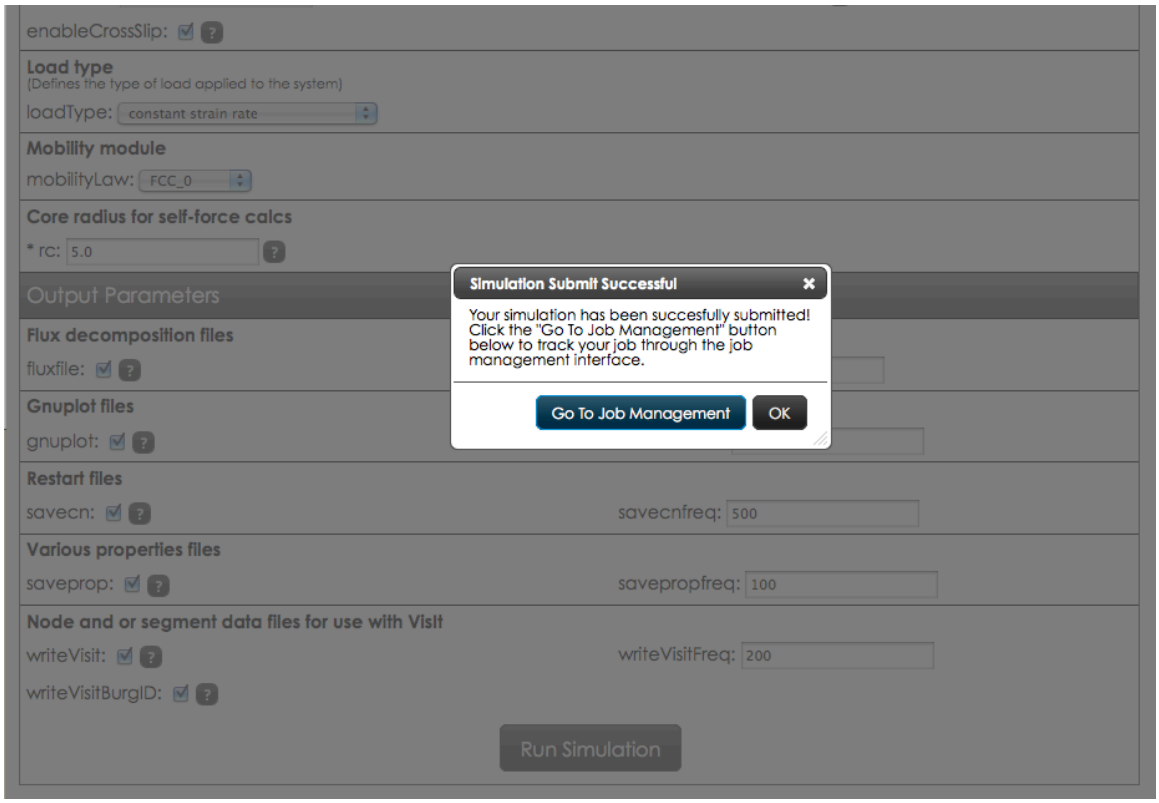
Attachment 4: Lorenz Screenshots



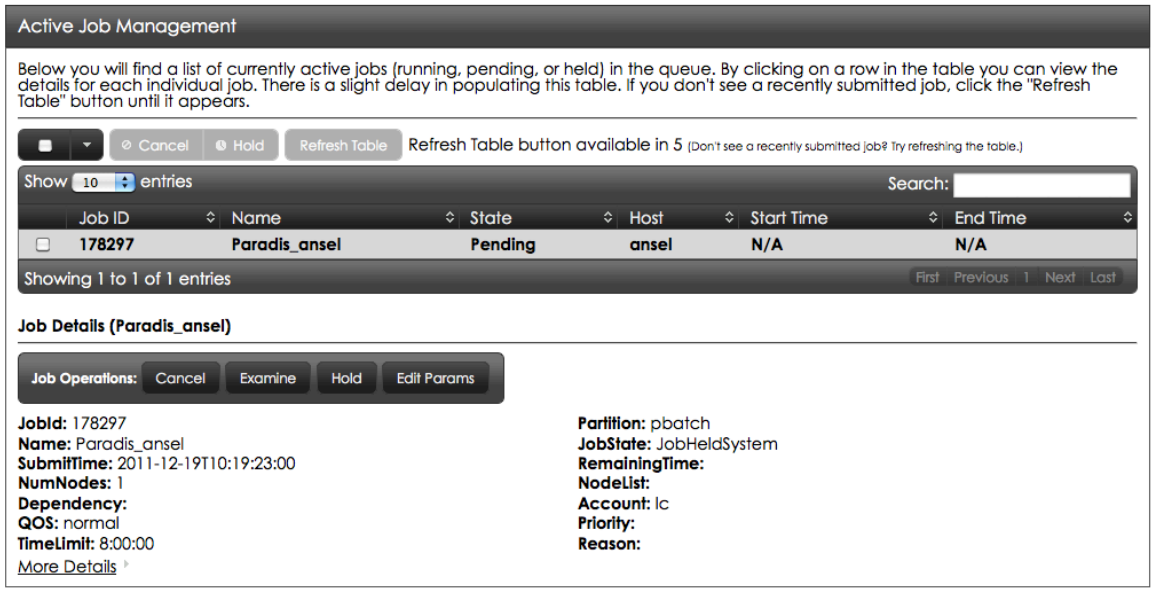
Screen capture of the simulation selector, part of the Lorenz Application Portal.



Screen capture of Lorenz simulation interface for ParaDiS, with copper option.



Screen capture of Lorenz response after submitting simulation.



Screen capture of Lorenz job management page showing job submitted via the Application Portal